Letters to the Editor

The Board of Editors will not hold itself responsible for opinions expressed in the letters, published in this section. The notes containing reports of new work communicated for this section should not contain many figures and should not exceed 500 words in length. The contributions must reach the Assistant Editor not later than the 15th of the second month preceding that of the issue in which the Letter is to appear. No proof will be sent to the authors.

8. SOFT X-RAY EMISSION SPECTROSCOPY OF GRAPHITE AND THE SUGGESTION OF A SUITABLE BRILLOUIN ZONE FOR IT.

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Three different Brillouin zones for graphite have, from time to time, been proposed by different workers (Ganguli and Krishnan, 1941; Wallace, 1947; Dutta, 1957) the details of which are given in the table below.

No. of electrons that can be contained in the Brillouin zone	Boundary planes	Structure factor for the boundary planes	Value of K, the reciprocal lattice vector for the boundary planes in 10^8 cm^{-1}	Fermi energy calculated according to the simple Sommerfeld formula in electron volts
1	$\bar{1}\bar{1}0, 0$	1	1.47	8.4
	000, 2	4	0 92	
3	$\bar{2}\bar{1}1, 0$	4	2.55	17 6
	000, 2	4	0.92	
4	220, 0	1	2.95	22
	000, 2	4	0.92	

It is well known that soft X-ray emission spectrum can furnish direct evidences regarding the band structure of solids and an attempt is made here to utilise the available data to decide the proper Brillouin zone in graphite. The variation on $N(E)$, the density of state with E, the energy within a Brillouin zone has been obtained in the case of graphite from its soft X-ray spectroscopy by Skinner (1940) and is repersented in the adjoining graph. The nature of variation of $N(E)$ with E is obviously that of a semimetal (Wilson, 1954)—the first peak from the left hand side indicating the touching of a set of Brillouin zone boundaries which, in view of the kink following, has evidently been overlapped ; the second peak indicating the maximum energy up to which the levels are filled under the normal state of the lattice as well as the contiguity of another set of bounding planes of Brillouin zone. The $N(E)$ value then falls rather sharply, the absorption edge lying near about the lowest point of this curve. The total band width is therefore about 24 ± 3 ev. From the above, the essential requirements of the proper Brillouin zone of graphite are : (i) it should be bounded by two independent sets of planes, one such set being overlapped; (ii) band width between

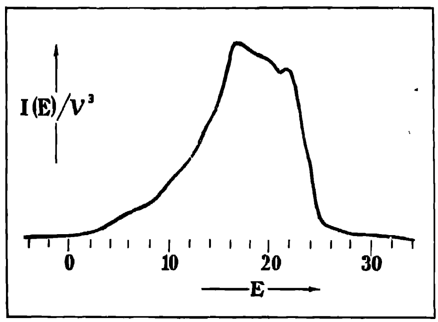

Fig. 1.—Intensity distribution of the soft X-ray emission spectra of graphite.

$I(E)$ = intensity in numbers of quanta per second of radiation in the emitted band in the unit range of quantum energy.

ν = absolute energy of transition

E = energy in electron volts ($\pm$ 3).

one set of planes should be much greater than that between the other set; (iii) the total band width should be about 24 ± 3 ev. On a reference to the table above it is evident that the one electron zone satisfies the requirements (i) and (ii), the three electron zone satisfies only (ii) and the four electron zone satisfies all the three conditions. Therefore, the four electron zone may now be considered to be the most suitable one for graphite. This acceptance of the four electron zone for graphite is further supported by the following essential considerations :

(1) It can be shown from a consideration of the nature of variation of $N(E)$ with E, the peculiar crystal structure of graphite and the electronic specific heat of graphite that 16 ev representing the position of the first peak from the left hand side correspond to a K-value equal to that for the $(2\bar{2}0, 0)$ planes. The band width between the kink and the absorption edge can also be shown to correspond to a K-value equal to that for the (000, 2) planes.

(2) The existence of π- and σ- electron interaction in the C-C bond formation in graphite which is also a necessary requirement of the acceptance of the 4-electron Brillouin zone has been proved amongst others by Coulson (1951 and 1952), Altman (1952) and others (March, 1952), Pariser (1953), Niira (1952), Davies, Hirschfelder and others (1955).

The details of these discussions have been dealt with in a separate paper and is in course of publication elsewhere.

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